

Inverse problem for the Landau-Zener effect

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Abstract. – We consider the inverse Landau-Zener problem which consists in finding the energy-sweep functions $W(t) \equiv \varepsilon_1(t) - \varepsilon_2(t)$ resulting in the required time dependences of the level populations for a two-level system crossing the resonance one or more times during the sweep. We find sweep functions of particular forms that let manipulate the system in a required way, including complete switching from the state 1 to the state 2 and preparing the system at the exact ground and excited states at resonance.

The Landau-Zener (LZ) effect [1, 2, 3], which consists in the quantum-mechanical transition between the two time-dependent levels of a two-level system (states 1 and 2) caused by crossing the resonance, is a well known phenomenon in many areas of physics. Well known applications of the LZ effect are those to molecular collision and dissociation [4, 5]. Recently, LZ effect has been used to measure the tunnel splitting in molecular magnets whereby detecting topological interference effects [6] which were predicted theoretically [7, 8, 9]. If the system was in state 1 before crossing the resonance, then, for a constant sweep rate v , the probability to stay in this state after crossing the resonance is given by

$$P = \exp\left(-\frac{\pi\Delta^2}{2\hbar v}\right), \quad (1)$$

where $v \equiv |\dot{W}(t)|$, $W(t) \equiv \varepsilon_1(t) - \varepsilon_2(t)$, $\varepsilon_{1,2}(t) = \langle \psi_{1,2} | \hat{H} | \psi_{1,2} \rangle$, $\Delta \equiv 2\langle \psi_1 | \hat{H} | \psi_2 \rangle$, $W(t)$ satisfies $W(\pm\infty) = \pm\infty$ and Δ is the tunnel level splitting. For *fast* energy sweep rates v the system spends too little time in the vicinity of the resonance so that the tunneling matrix element $\langle \psi_1 | \hat{H} | \psi_2 \rangle$ cannot bring the system into the state 2 (say, onto the other side of a potential barrier), and the system remains in the initial state 1. For *slow* sweep rates the probability to remain in the initial state becomes exponentially small, and the system travels into the state 2 remaining on the lower *exact* energy term $\varepsilon_-(t)$ of

$$\varepsilon_{\pm}(t) = \frac{1}{2} \left[\varepsilon_2(t) + \varepsilon_1(t) \pm \sqrt{W^2(t) + \Delta^2} \right]. \quad (2)$$

The corresponding *adiabatic* time dependence of the probability to be in state 1 is given by

$$|c_1(t)|^2 = |\langle \psi_1 | \psi_-(t) \rangle|^2 = \frac{1}{2} \left(1 - \frac{W(t)}{\sqrt{W^2(t) + \Delta^2}} \right). \quad (3)$$

In the case where $\hbar v \sim \Delta^2$ and v is constant, the solution of the Schrödinger equation for $|c_1(t)|^2$ can be found analytically [1, 2, 3] and it is oscillating at $t > 0$ slowly approaching P given by Eq. (1) at $t \rightarrow \infty$.

The known results above are valid for the linear energy sweep, $W(t) = vt$. One can consider, however, other sweep functions $W(t)$ that behave *nonlinearly* in the vicinity of the resonance, $W \sim \Delta$. If the tunneling resonance is not too narrow and its position is well defined, nonlinear sweeps of a controlled form can be realized experimentally. Although no general analytical solution of the Schrödinger equation is known for the LZ problem with an arbitrary $W(t)$, one can look for the functions $W(t)$ that result in a desired time dependence of the probability $|c_1(t)|^2$, thus solving the *inverse* LZ problem. It is the main motivation of this Letter to study this inverse problem which, for instance, will allow to determine $W(t)$ needed to manipulate and to prepare a quantum system in a specific state.

One class of solutions of the time-dependent Schrödinger equation are smooth, non-oscillating functions of time that describe the complete switching of the system from the state 1 to the state 2, e.g., Eq. (3). Another class of solutions are those starting in ψ_1 at $t = -\infty$ off resonance and ending in a given superposition of the exact states ψ_{\pm} at resonance [$W(t) = 0$ for $t \geq 0$]. The most interesting variants of the latter are the system in the ground state ψ_- at resonance and in the excited state ψ_+ at resonance. These possibilities to manipulate the system in a required way could prove to be useful for the quantum computing (QC). Another interesting possibility is to sweep at a high rate (nonlinearly in time) far from the resonance thus making the whole process of crossing the resonance much shorter. Exploring these new types of solution of the LZ problem is the aim of this Letter.

To this end, we consider the Schrödinger equation for the coefficients in the wave function $\psi(t) = c_1(t)\psi_1 + c_2(t)\psi_2$ that can be written in the form

$$\begin{aligned} \hbar \dot{p}(t) &= -\frac{i}{2}\Delta q(t), & p(-\infty) &= 1 \\ \hbar \dot{q}(t) &= iW(t)q(t) - \frac{i}{2}\Delta p(t), & q(-\infty) &= 0, \quad W(-\infty) = -\infty \end{aligned} \quad (4)$$

with $p(t) \equiv e^{i\varepsilon_1 t} c_1(t)$ and $q(t) \equiv e^{i\varepsilon_2 t} c_2(t)$. We are looking for sweep functions $W(t)$ that result in a required time dependence of the state populations. Before solving this inverse LZ problem analytically, we will illustrate numerically the possibility of time-symmetric solutions of Eq. (4) going from $p(-\infty) = 1$ to $p(\infty) = 0$ for strongly nonlinear sweep functions $W(t)$. The simplest of these cases is the cubic-parabola sweep with $W(t) = -2.5t + 1.83t^3$ where we have set $\Delta = \hbar = 1$ in Eq. (4). The time dependence of the probability $|p(t)|^2$ shown in Fig. 1 can be fitted by $|p|^2(t) = [1 - \tanh(\sinh(t))]/2$ which is, however, not the analytical solution of Eq. (4).

To find analytical solutions of the inverse LZ problem, one should rewrite Eq. (4) in terms of the probability $m \equiv |p|^2$ and some phase variable. We thus define

$$p = \sqrt{m} \exp(i\varphi_p), \quad q = \sqrt{1-m} \exp(i\varphi_q) \quad (5)$$

and substitute it in Eq. (4). Evidently the global phase of the system $(\varphi_p + \varphi_q)/2$ is irrelevant and the resulting Schrödinger equation can be formulated in terms of m and the phase difference $\varphi = \varphi_q - \varphi_p$:

$$\begin{aligned} \hbar \dot{m} &= \Delta \sqrt{m(1-m)} \sin \varphi \\ \hbar \dot{\varphi} &= W + \frac{\Delta}{2} \frac{1-2m}{\sqrt{m(1-m)}} \cos \varphi. \end{aligned} \quad (6)$$

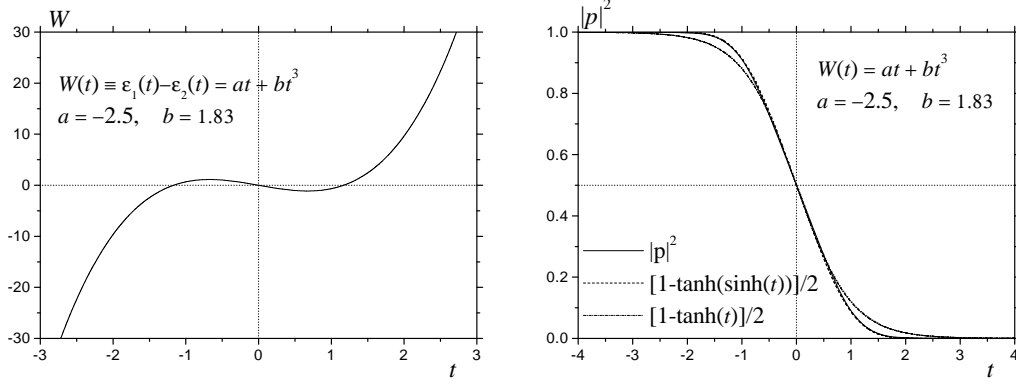


Fig. 1. – The cubic-parabola energy sweep with $W(t) = -2.5t + 1.83t^3$ and $\Delta = \hbar = 1$. Time dependence of the probability $|c_1(t)|^2 = |p(t)|^2$ can be fitted with $|p|^2 = [1 - \tanh(\sinh t)]/2$ with graphic accuracy. The function $|p|^2 = [1 - \tanh t]/2$ is shown for comparison.

This system of equations can be brought into a more elegant form by introducing

$$x \equiv 2m - 1, \quad -1 < x < 1, \quad (7)$$

$$y \equiv \arcsin x, \quad -\pi/2 < y < \pi/2, \quad (8)$$

and the reduced variables

$$\tau \equiv (\Delta/\hbar)t, \quad \overline{W} \equiv W/\Delta. \quad (9)$$

Then Eqs. (6) can be put into the reduced form

$$\begin{aligned} \partial_\tau y &= \sin \varphi \\ \partial_\tau \varphi &= \overline{W} - \tan y \cos \varphi. \end{aligned} \quad (10)$$

The boundary condition for this equation is $y(-\infty) = \pi/2$ whereas the value of $\varphi(-\infty)$ is irrelevant. In general, far from the resonance $\varphi(\tau)$ strongly oscillates with time and the derivative $\partial_\tau y$ is not small. Below we will consider special kinds of solutions of Eq. (10) which are characterized by a smooth, non-oscillating dependence $\sin \varphi(\tau)$ and $\partial_\tau y(-\infty) = 0$. We will solve the inverse problem for Eq. (10) which consists in finding $\overline{W}(\tau)$ resulting in a required function $x(\tau)$. One easily obtains from Eq. (10) a general formula

$$\overline{W}(\tau) = \partial_\tau \varphi + \tan y \cos \varphi = \partial_\tau^2 y / \cos \varphi + \tan y \cos \varphi, \quad \cos \varphi = \pm \sqrt{1 - (\partial_\tau y)^2}. \quad (11)$$

The sign in front of $\cos \varphi$ determines the sign of the function $\overline{W}(\tau)$. Since $|c_1(-\infty)|^2 = 1$ and thus $x(-\infty) = 1$ and $y(-\infty) = \pi/2$ one has $\tan y(-\infty) = \infty$. To comply with the condition $W(-\infty) = -\infty$ one has to choose, in general, the negative sign:

$$\overline{W}(\tau) = -\partial_\tau^2 y / \sqrt{1 - (\partial_\tau y)^2} - \tan y \sqrt{1 - (\partial_\tau y)^2}. \quad (12)$$

Before considering particular cases, we will comment on some general properties of the functions $x(\tau)$ and $\overline{W}(\tau)$. If $x(\tau)$ is an odd function of time then y is also odd and $\partial_\tau y(\tau)$ is even, whereas $\partial_\tau^2 y(\tau)$ and $\tan y(\tau)$ are odd. Then from the first of Eqs. (10) follows that $\sin \varphi(\tau)$ is even. If the sign of $\cos \varphi$ does not change, which is the generic situation, $\cos \varphi(\tau)$

is even. Then from Eq. (11) follows that $\overline{W}(\tau)$ is odd. In a similar way one can show that if $x(\tau)$ is even (the system returns into the initial state ψ_1 after crossing the resonance) then $\overline{W}(\tau)$ is even, too.

There is an important special case, however, which is realized if the derivative $\partial_\tau y$ at some point τ_0 attains its *maximal* value $|\partial_\tau y| = 1$ which follows from the first of Eqs. (10). At this point $\cos \varphi$ turns to zero and changes its sign to positive. The latter corresponds to the phase φ going from the interval $\pi/2 < \varphi < \pi$ into the interval $0 < \varphi < \pi/2$. Note that $\partial_\tau^2 y = 0$ at $\tau = \tau_0$ thus Eq. (12) does not diverge. If $\tau_0 = 0$ then $\cos \varphi(\tau)$ is an odd function: $\cos \varphi < 0$ for $\tau < 0$ and $\cos \varphi > 0$ for $\tau > 0$. As a result, the parity of $\overline{W}(\tau)$ becomes inverse to the parity of $x(\tau)$. If $\tau_0 \neq 0$ then for a symmetric function $x(\tau)$ the similar happens at $\tau = -\tau_0$. That is, $\cos \varphi(\tau)$ changes sign two times and is an even function, thus the parity of $\overline{W}(\tau)$ coincides with that of $x(\tau)$. It should be noted that parity considerations for the direct LZ problem do not apply: Symmetric forms of $\overline{W}(\tau)$ do not necessarily result in symmetric solutions $x(\tau)$. If, however, the solution $x(\tau)$ satisfies $x(\pm\infty) = \mp 1$ or $x(\pm\infty) = \pm 1$ and $\overline{W}(\tau)$ is time symmetric, then $x(\tau)$ is also symmetric. This follows from the time reversibility of the Schrödinger equation and the symmetry of the boundary values of $x(\tau)$.

Another implication of this analysis is the existence of the *maximal* rate of the probability change. We have seen that $|\partial_\tau y| \leq 1$, then from $\partial_\tau x = \sqrt{1-x^2} \partial_\tau y$ follows $|\partial_\tau x| \leq 1$. This limitation is physically clear: Since tunneling between ψ_1 and ψ_2 is caused by the matrix element $\Delta \equiv 2\langle\psi_1|\hat{H}|\psi_2\rangle$, the latter sets up the natural scale for the tunneling rate, see Eq. (9). To completely tunnel from ψ_1 to ψ_2 , the system should spend some minimal time in the vicinity of the resonance, that is, the sweep cannot be too fast. Below we will discuss two most important families of the functions $x(\tau)$ and corresponding $\overline{W}(\tau)$ which depend on τ in the combination $u = a\tau$, the parameter a being the measure of the sweep rate. We will see that there is a maximal value $a = a_{\max}$ for which $|\partial_\tau y| = 1$ at some $\tau = \tau_0$. We will also see that although the functions $x(\tau)$ do formally exist for $a > a_{\max}$, one cannot extend $\overline{W}(\tau)$ into this region, as a result of the physical limitation on the tunneling rate. Thus solutions $x(\tau)$ with $a > a_{\max}$ are not realizable.

One of possible solutions is of the form

$$x = (-1)^n \frac{u^n}{\sqrt{1+u^{2n}}}, \quad u \equiv a\tau. \quad (13)$$

For n odd it describes switching of the probability from ψ_1 to ψ_2 , whereas for n even the system returns into the initial state. For $n = 1$ the form of Eq. (13) corresponds to Eq. (3) by taking into account Eq. (7) with $m = |c_1|^2$. However, the reader should note that Eq. (3) is realized with the very slow sweep $\overline{W}(\tau)$ of an arbitrary functional form, whereas Eq. (13) is valid for a particular form of $\overline{W}(\tau)$ which is not necessarily slow. One obtains from Eqs. (8) and (13)

$$\begin{aligned} \partial_\tau y &= \frac{1}{\sqrt{1-x^2}} \partial_\tau x = (-1)^n \frac{anu^{n-1}}{1+u^{2n}} \\ \partial_\tau^2 y &= (-1)^n \frac{a^2 nu^{n-2} [n-1-(n+1)u^{2n}]}{(1+u^{2n})^2}, \end{aligned} \quad (14)$$

whereas $\tan y = x/\sqrt{1-x^2} = (-1)^n u^n$. The derivative $\partial_\tau y$ has a chance to attain the value 1 at its maximum that is determined by $\partial_\tau^2 y = 0$, i.e., at

$$u = u_{\max} = \pm \left(\frac{n-1}{n+1} \right)^{1/(2n)}. \quad (15)$$

At this point one has

$$|(\partial_\tau y)_{\max}| = \begin{cases} a, & n = 1 \\ a^{\frac{n+1}{2}} \left(\frac{n-1}{n+1}\right)^{(n-1)/(2n)}, & n > 1, \end{cases} \quad (16)$$

thus the condition

$$a \leq a_{\max} = \begin{cases} 1, & n = 1 \\ \frac{2}{n+1} \left(\frac{n-1}{n+1}\right)^{2n/(n-1)}, & n > 1 \end{cases} \quad (17)$$

should be fulfilled. For $a < a_{\max}$ Eq. (12) yields

$$\overline{W}(\tau) = \frac{(-1)^{n-1} u^n}{\sqrt{1 - [anu^{n-1}/(1+u^{2n})]^2}} \left[1 - \frac{a^2 n [(2n+1)u^{2n-2} - (n-1)u^{-2}]}{(1+u^{2n})^2} \right], \quad u = a\tau. \quad (18)$$

This function is plotted for $n = 1$ and $n = 5$ and different values of the parameter a in Figs. 2a and 2b. For $a \rightarrow a_{\max}$ discontinuities in Eq. (18) are formed at $u = \pm u_{\max}$. These discontinuities result from the invariably negative choice for $\cos \varphi$. For $a = a_{\max}$ the sign of $\cos \varphi$ can change at $u = u_{\max}$ and then these discontinuities disappear. This form of $\overline{W}(\tau)$ includes the factor $\text{sgn} [(1+u^{2n})^2 - (anu^{n-1})^2]$, in addition to Eq. (18). Note that Eq. (18) cannot be extended into the region $a > a_{\max}$ preserving $\overline{W}(\tau)$ real, in contrast to Eq. (13). The small- and large-argument forms of $\overline{W}(\tau)$ are

$$\overline{W}(\tau) \propto (-1)^{n-1} \begin{cases} u^n, & |u| \gg 1 \\ u^{n-2}, & |u| \ll 1, \end{cases} \quad n > 1. \quad (19)$$

In the case $n = 1$, Eq. (18) simplifies to

$$\overline{W}(\tau) = \frac{u}{1+u^2} \frac{1-3a^2+2u^2+u^4}{\sqrt{1-a^2+2u^2+u^4}}. \quad (20)$$

One can see that for $u \gg 1$ the function $\overline{W}(\tau)$ describes a linear energy sweep with the velocity $v = a$. For $u \sim 1$ the form of $\overline{W}(\tau)$ is nonlinear and for $a < a_{\max} = 1$ the resonance is crossed three times, including $u = 0$. For $a = 1$ Eq. (20) yields the even function

$$\overline{W}(\tau) = \frac{2-2\tau^2-\tau^4}{(1+\tau^2)\sqrt{2+\tau^2}} \quad (21)$$

This sweep crosses the resonance two times, in the forward and backward directions, which means that the system is in the *excited* state ψ_2 at the end of the sweep at $t = \infty$. For $a < 1$ and far from the resonance Eq. (20) has the form

$$W(t) = \Delta \overline{W}(\tau) = \Delta a \tau = (\Delta^2 a / \hbar) t, \quad (22)$$

thus the corresponding linear sweep rate is $v = \Delta^2 a / \hbar$. The maximal sweep rate that ensures the complete switching to ψ_2 is realized at $a = 1$ is $v_{\max} = \Delta^2 / \hbar$. For a comparison, in the regular LZ effect with the probability to stay in the initial state given by Eq. (1) the sweep rate $v \ll \pi \Delta^2 / (2\hbar)$ is required for a complete switching. For $v = \Delta^2 / \hbar$ the probability to stay in the initial state is still $P = 0.208$.

Another solution that describes switching from state 1 to state 2 is

$$x = -\tanh u, \quad u = a\tau. \quad (23)$$

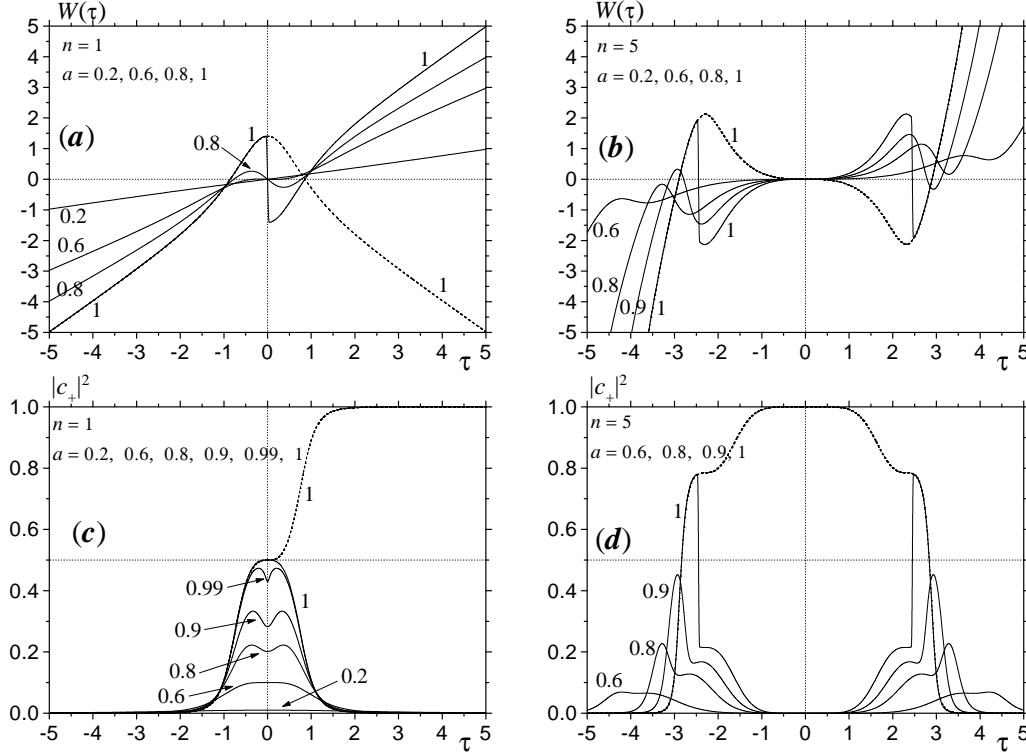


Fig. 2. – *a* – Energy sweep function $\overline{W}(\tau)$ of Eq. (18) with $n = 1$ [or of Eq. (20)] for different values of the sweep rate a . *b* – The same with $n = 5$. *c* – The population of the exact excited level, $|c_+|^2$, for $n = 1$ and different values of a . *d* – The same for $n = 5$. Dashed lines in all graphs correspond to $a = a_{\max}$ and $\overline{W}(\tau)$ without jumps [see, e.g., Eq. (21)].

Here the sweep function determined from Eq. (12) reads

$$\overline{W}(\tau) = \frac{\sinh u}{\sqrt{1 - a^2/\cosh^2 u}} \left[1 - \frac{2a^2}{\cosh^2 u} \right]. \quad (24)$$

In the range $1/\sqrt{2} < a < 1$ the function $\overline{W}(\tau)$ changes its sign three times and its derivative at $\tau = 0$ is negative. With $a \rightarrow 1$ this derivative increases unlimitedly and a jump of $\overline{W}(\tau)$ at $\tau = 0$ is formed. For $a = a_{\max} = 1$ the solution with eliminated jump is an even function

$$\overline{W}(\tau) = \frac{2}{\cosh \tau} - \cosh \tau. \quad (25)$$

This sweep function crosses the resonance two times. Again, Eq. (24) cannot be continued into the region $a > 1$.

Now we return to the solution for the probability x described by Eq. (13) and analyze its behavior for large n . It has a form of three plateaus $x \cong 1$ for $u \lesssim -1$, $x \cong 0$ for $-1 \lesssim u \lesssim 1$, and $x \cong -1$ for $1 \lesssim u$ with two narrow transition regions between them. In the central region $-1 \lesssim u \lesssim 1$ one has $|c_2|^2 \cong |c_1|^2 = (1+x)/2 \cong 1/2$, i.e., the system is in the mixture of the states ψ_1 and ψ_2 with equal weights. The sweep function $\overline{W}(\tau)$ of Eq. (18) is fast approaching the resonance at $u \cong -1$ and remaining in the close vicinity of the latter until $u \cong 1$. Since

the probabilities $|c_1|^2 \cong |c_2|^2 \cong 1/2$ do not oscillate in the range $-1 \lesssim u \lesssim 1$ (unlike the case in which the system is instantaneously brought into resonance), one is lead to the conclusion that the system is in one of the exact quantum states ψ_- or ψ_+ . It is naturally of interest to question in which of these exact states does the system come under the influence of the energy sweep described by Eq. (18). We will see below that both variants can be realized. This opens a possibility to prepare the system in the ground or excited state in resonance by the appropriate choice of $\overline{W}(\tau)$. Indeed, for $n \geq 3$ one has $\overline{W}(\tau) = \partial_\tau y = \partial_\tau^2 y = 0$ at $\tau = 0$, thus from Eq. (10) one can see that the sweep can be stopped at $\tau = 0$ and the system will remain in this state. To demonstrate this behavior one should rewrite the wave function of the system $\psi = c_1(t)\psi_1 + c_2(t)\psi_2$ determined above in the basis of the exact states

$$\psi_\pm(t) = \frac{1}{\sqrt{2}} [\pm K_\pm(t)\psi_1 + K_\mp(t)\psi_2], \quad K_\pm(t) \equiv \sqrt{1 \pm \frac{\overline{W}(t)}{\sqrt{1 + \overline{W}^2(t)}}} \quad (26)$$

corresponding to the time-dependent “energy eigenvalues” of Eq. (2) as $\psi = c_+(t)\psi_+(t) + c_-(t)\psi_-(t)$. The corresponding probabilities are given by

$$|c_\pm(t)|^2 = \frac{1}{2} \left\{ 1 \pm \frac{\overline{W}(t)x(t) + \sqrt{1 - x^2(t)} \cos \varphi(t)}{\sqrt{1 + \overline{W}^2(t)}} \right\}. \quad (27)$$

One can see that in resonance at $t = 0$ ($\overline{W} = x = 0$, $\cos \varphi = \pm 1$) the situation depends on the sign of $\cos \varphi$. For sweep functions given by Eq. (18) with $a < a_{\max}$ one has $\cos \varphi = -1$ and the system is in the ground state ($|c_-(t)|^2 = 1$, $|c_+(t)|^2 = 0$). For the special sweep functions with $a = a_{\max}$ one has $\cos \varphi = 1$ and the system is in the excited state ($|c_-(t)|^2 = 0$, $|c_+(t)|^2 = 1$), the transition from the ground state $\psi_-(t)$ to the excited state $\psi_+(t)$ occurring for $n \gg 1$ in the vicinity of $u = u_{\max}$ of Eq. (15). These features are illustrated for the sweep functions of Eqs. (18) and (21) in Figs. 2c and 2d. Note that for $n = 1$ and $a = a_{\max} = 1$ the sweep function of Eq. (21) returns to $-\infty$ at $\tau = \infty$ and the system ends up in the excited state $\psi_+ = \psi_2$.

To conclude, we have solved the inverse Landau-Zener problem for a two-level system, i.e., we have established the form of the sweep function $W(t) \cong \varepsilon_1(t) - \varepsilon_2(t)$ needed to insure a given probability $|c_1(t)|^2$ to be in the state 1 at time t . We have discussed two examples for which the system performs a *complete* transition from 1 to 2. In contrast to the direct LZ problem with a linear sweep, this can be accomplished by a *finite* sweeping rate. Further we have found such sweep functions that prepare the system in its exact ground state or in its exact excited state at resonance. It is not difficult to find $W(t)$ that prepare the system in an *arbitrary* mixture of the exact states at resonance, which can be potentially used in quantum computing based on tunneling units.

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